

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020422\
 Data File : BF126817.D
 Acq On : 04 Feb 2022 18:05
 Operator : CG/JU
 Sample : N1381-10
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DB-09(25-30)-02-02-22

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126817.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.299	28	36	42	rVB	451376	592302	13.11%	1.609%
2	3.163	176	183	190	rBB	31915	49631	1.10%	0.135%
3	5.198	525	529	536	rVB	46449	56296	1.25%	0.153%
4	5.569	587	592	595	rBV	4073906	4249115	94.07%	11.546%
5	6.569	755	762	769	rBV	3678991	4516867	100.00%	12.274%
6	6.945	822	826	829	rBV	1176071	908888	20.12%	2.470%
7	6.998	829	835	841	rBV	126036	112357	2.49%	0.305%
8	7.510	916	922	925	rBV	2966472	2910544	64.44%	7.909%
9	8.128	1024	1027	1034	rBV	50926	94402	2.09%	0.257%
10	8.228	1040	1044	1047	rBV	1471683	1181698	26.16%	3.211%
11	9.304	1222	1227	1230	rBV	4674375	4324827	95.75%	11.752%
12	9.575	1268	1273	1277	rBV	146404	145025	3.21%	0.394%
13	9.692	1290	1293	1296	rBV2	47006	46939	1.04%	0.128%
14	9.986	1339	1343	1346	rBV	1691018	1342235	29.72%	3.647%
15	10.304	1392	1397	1402	rBV	43410	83206	1.84%	0.226%
16	10.780	1473	1478	1481	rBV	2637905	2675056	59.22%	7.269%
17	10.886	1493	1496	1500	rVB2	43007	63265	1.40%	0.172%
18	11.480	1593	1597	1600	rBV	1528572	1346182	29.80%	3.658%
19	11.863	1658	1662	1665	rVB	640231	548744	12.15%	1.491%
20	11.986	1681	1683	1687	rBV	88208	85301	1.89%	0.232%
21	12.551	1775	1779	1780	rBV	1705486	1384341	30.65%	3.762%
22	12.574	1780	1783	1788	rVV	3933077	3850882	85.26%	10.464%
23	12.615	1788	1790	1794	rVV	99908	93338	2.07%	0.254%
24	12.657	1794	1797	1801	rVV	294686	242546	5.37%	0.659%
25	12.868	1830	1833	1837	rVB	122534	97235	2.15%	0.264%
26	13.068	1862	1867	1870	rBV	3937416	3541924	78.42%	9.624%
27	13.304	1905	1907	1910	rVB	71018	51594	1.14%	0.140%
28	14.092	2039	2041	2043	rBV	61498	46415	1.03%	0.126%
29	14.121	2043	2046	2050	rVB	889202	755540	16.73%	2.053%
30	14.439	2097	2100	2102	rVB	68861	57473	1.27%	0.156%
31	14.751	2149	2153	2157	rBV	188536	190012	4.21%	0.516%
32	14.904	2176	2179	2184	rVB	46258	48164	1.07%	0.131%
33	15.256	2236	2239	2245	rBV	50602	56087	1.24%	0.152%
34	15.639	2299	2304	2313	rVB2	574589	805015	17.82%	2.187%
35	16.121	2382	2386	2391	rVB2	40287	60772	1.35%	0.165%
36	16.656	2471	2477	2483	rBV3	38528	77200	1.71%	0.210%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.292	2581	2585	2596	rVB4	23559	53502	1.18%	0.145%
38	18.045	2707	2713	2723	rVB9	22446	56343	1.25%	0.153%

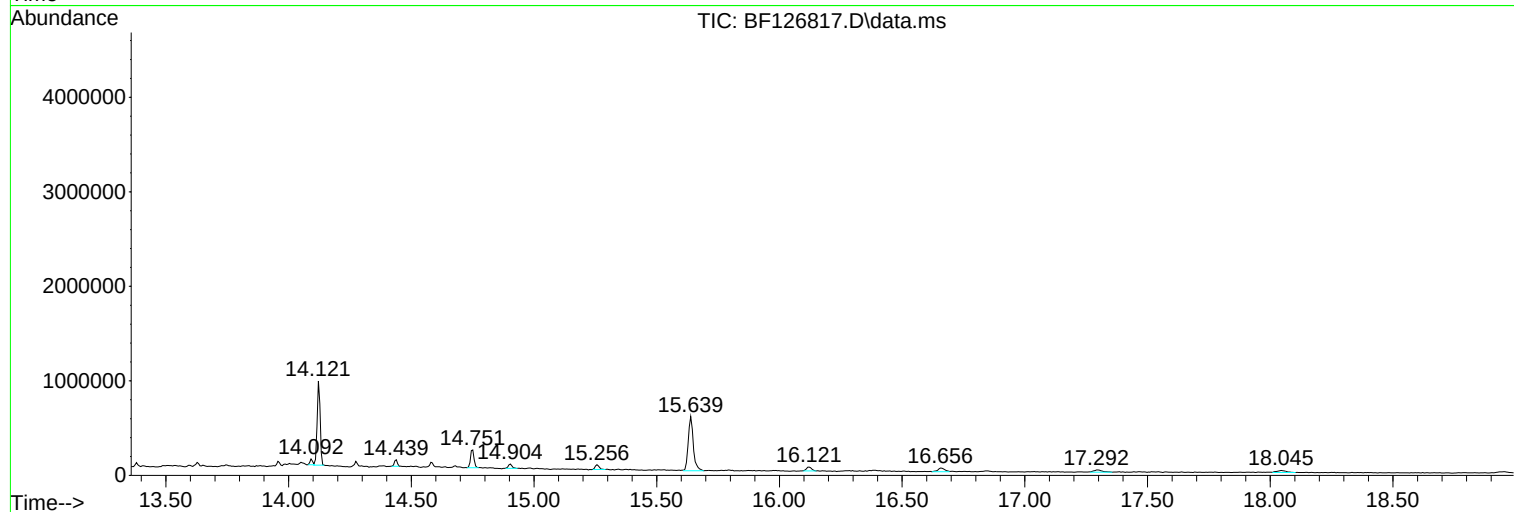
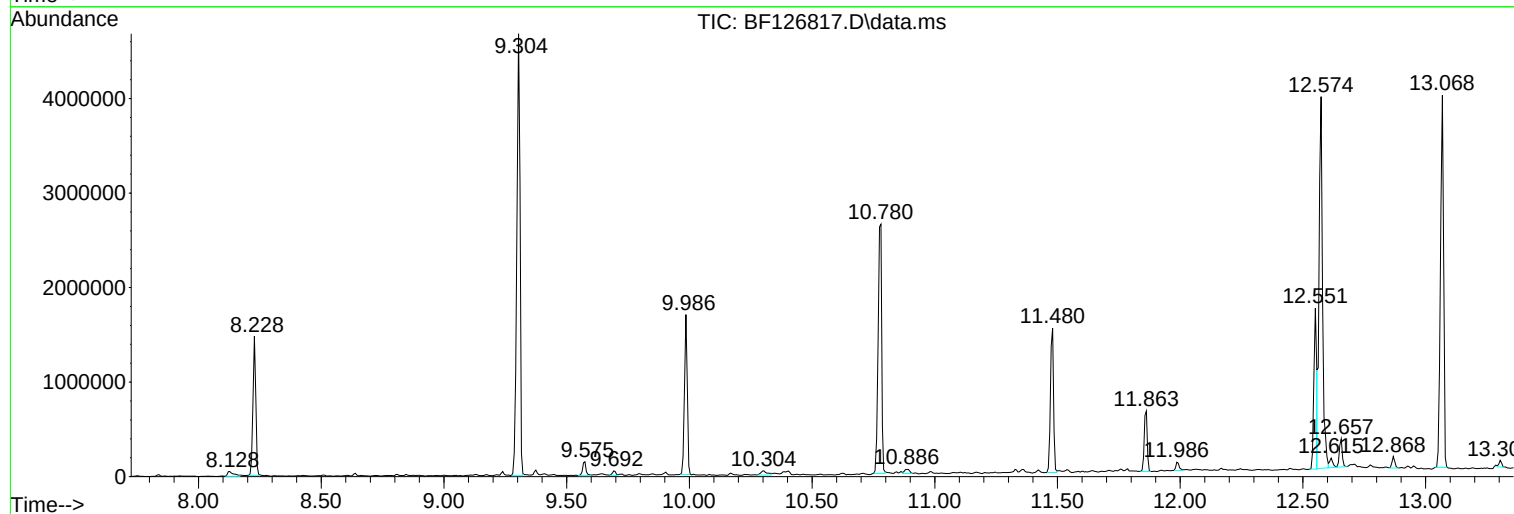
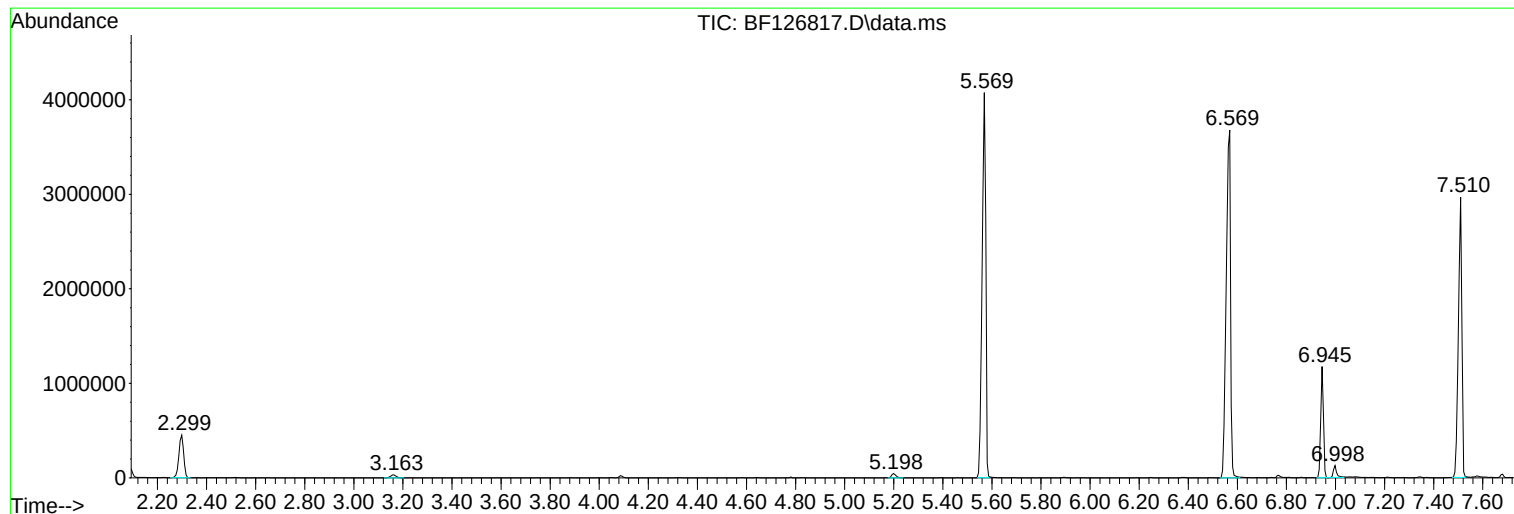
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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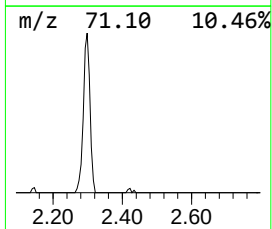
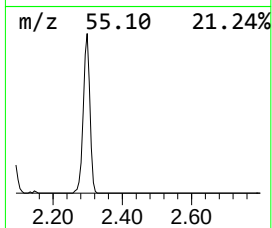
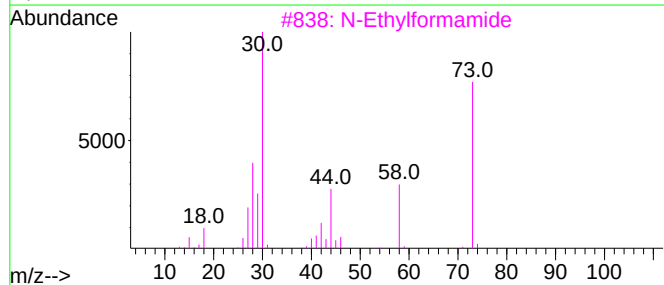
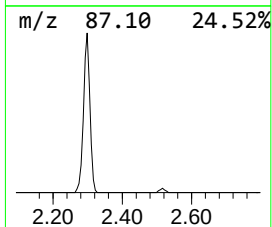
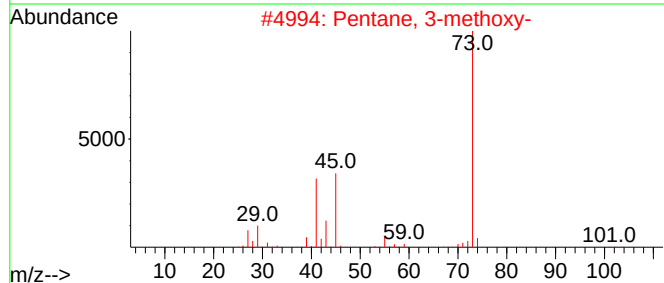
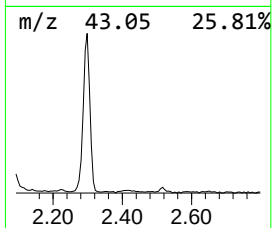
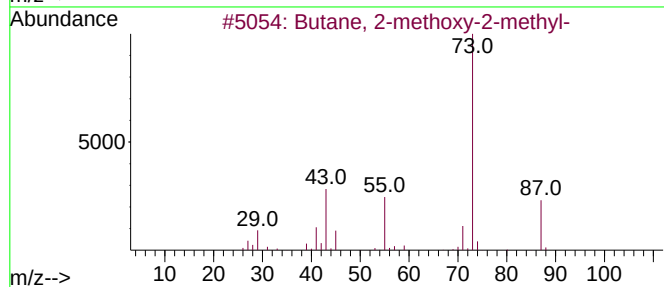
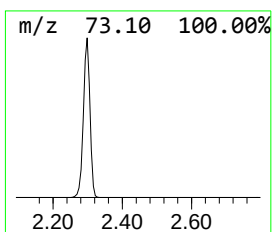
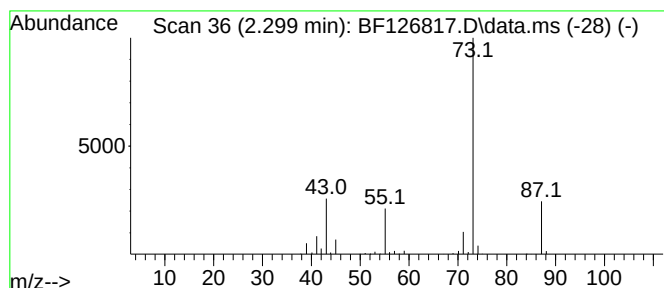
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.299	13.03 ng	592302	1,4-Dichlorobenzene-d4	6.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
3			N-Ethylformamide	73	C3H7NO	000627-45-2	9
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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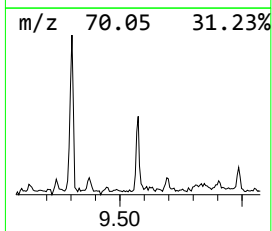
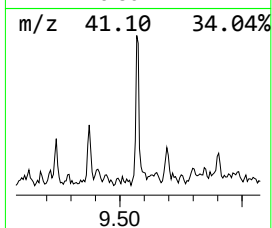
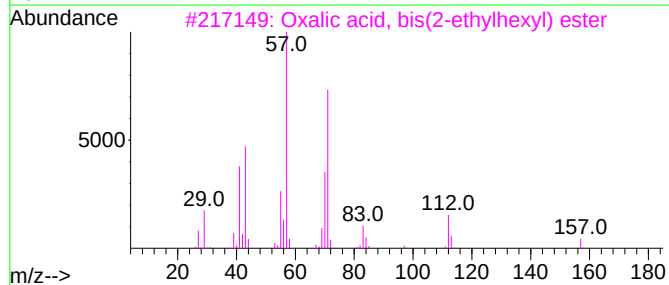
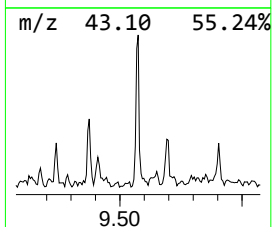
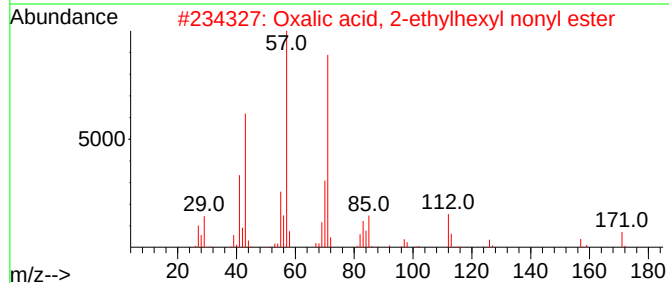
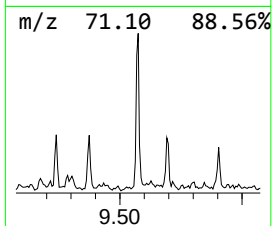
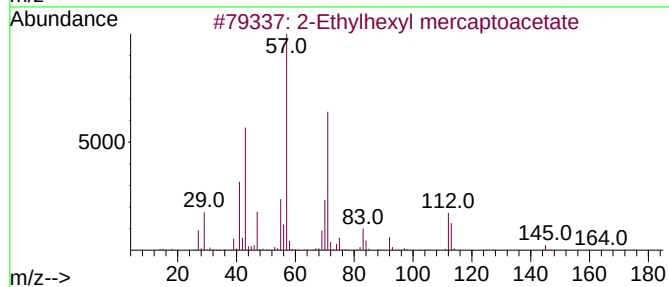
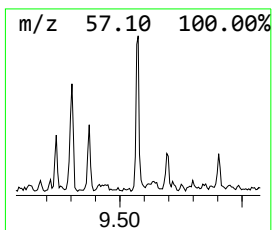
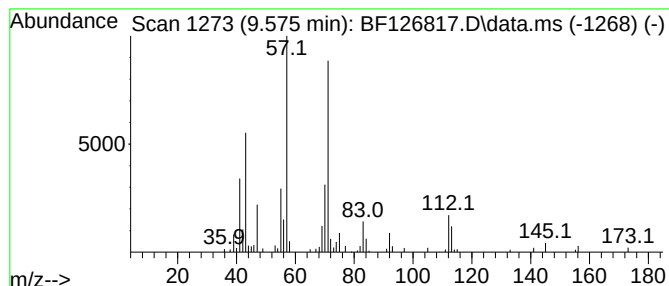
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Ethylhexyl mercaptoacetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.575	2.16 ng	145025	Acenaphthene-d10	9.986

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Ethylhexyl mercaptoacetate	204	C10H20O2S	007659-86-1	91
2			Oxalic acid, 2-ethylhexyl nonyl ...	328	C19H36O4	1000309-39-2	64
3			Oxalic acid, bis(2-ethylhexyl) e...	314	C18H34O4	1000309-39-0	64
4			Oxalic acid, 2-ethylhexyl ethyl ...	230	C12H22O4	1000309-38-4	64
5			Decane, 4-methyl-	156	C11H24	002847-72-5	62



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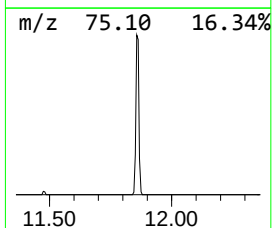
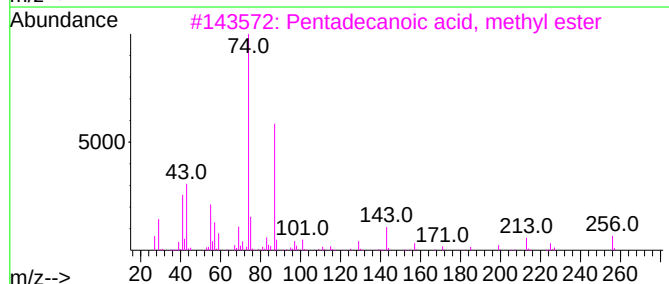
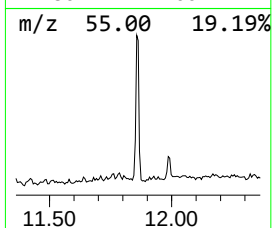
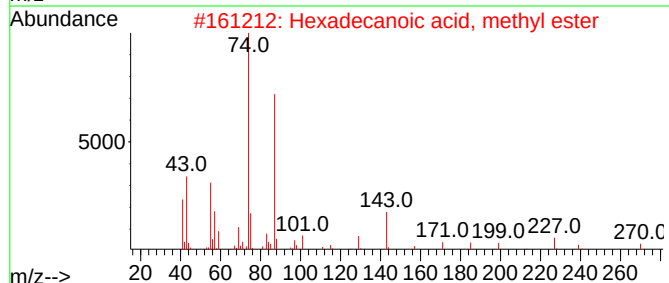
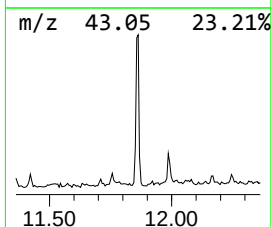
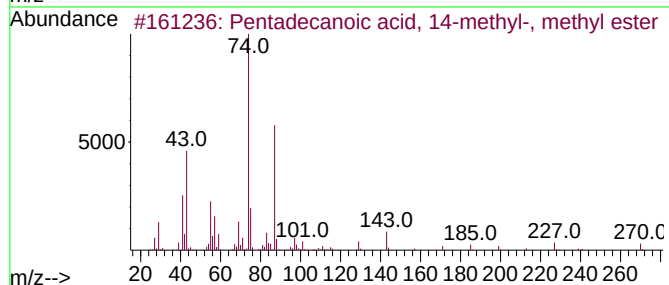
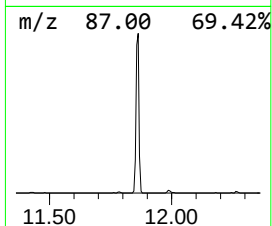
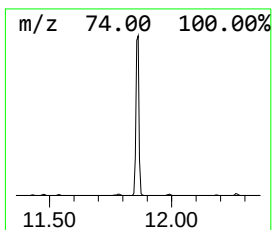
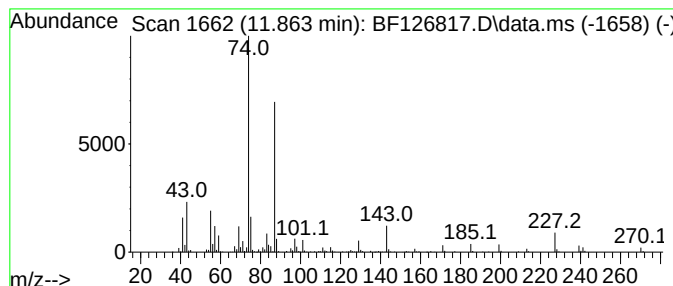
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentadecanoic acid, 14-meth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	8.15 ng	548744	Phenanthrene-d10	11.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	97
2			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	96
3			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4			Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	87
5			Methyl tetradecanoate	242	C15H30O2	000124-10-7	87



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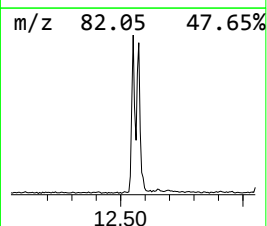
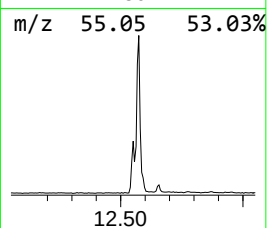
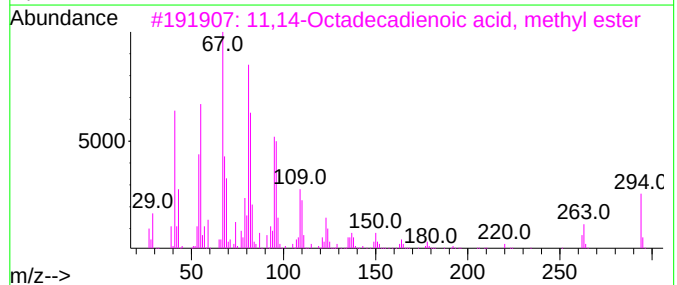
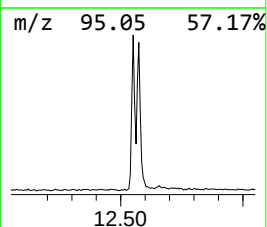
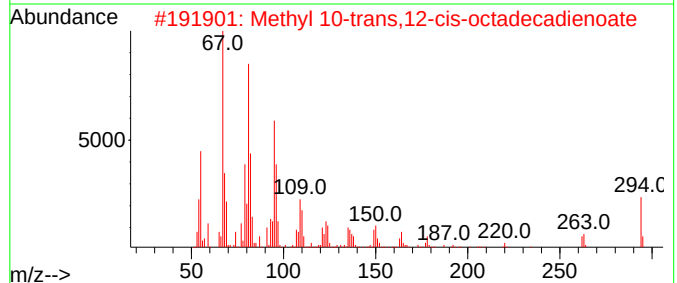
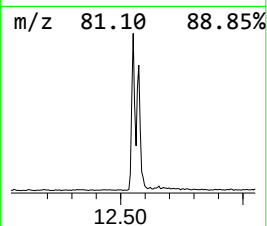
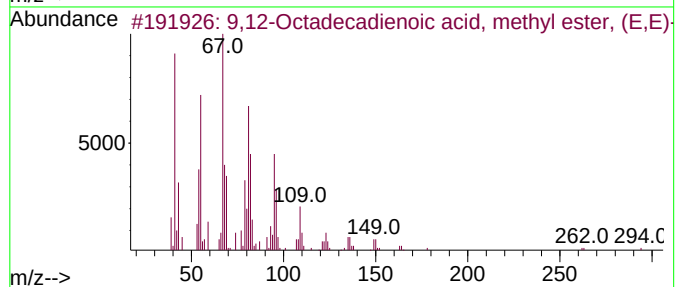
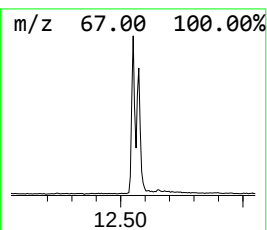
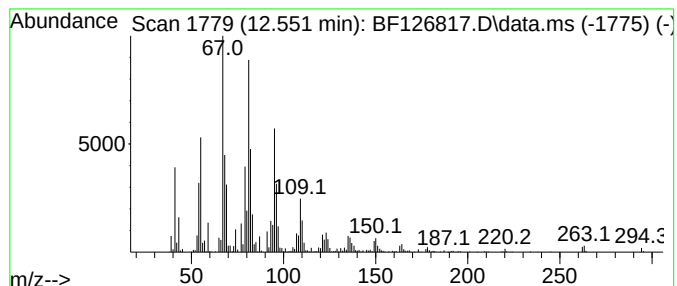
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Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.551	20.57 ng	1384340	Phenanthrene-d10	11.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2			Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	96
3			11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	96
4			9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	95
5			12,15-Octadecadienoic acid, meth...	294	C19H34O2	057156-97-5	93



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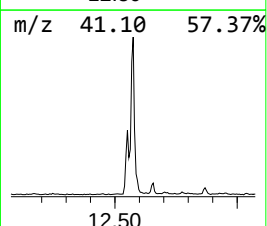
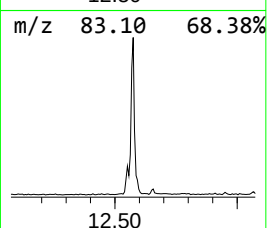
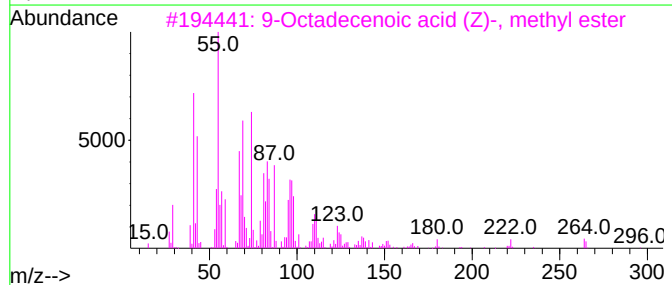
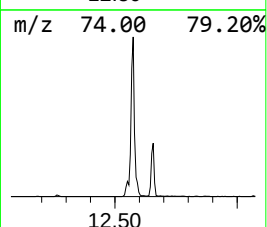
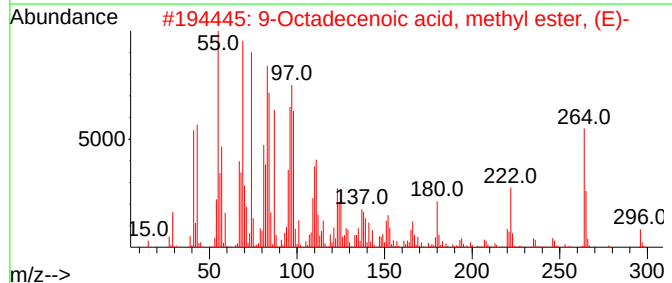
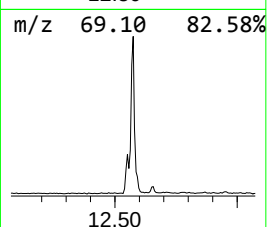
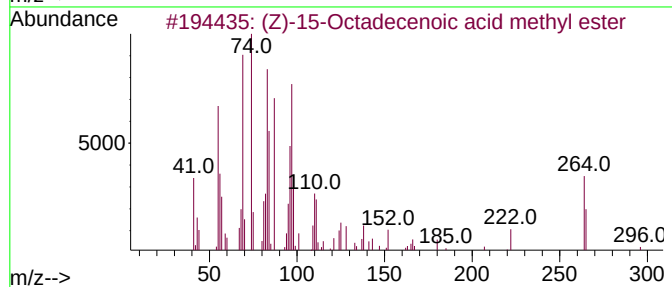
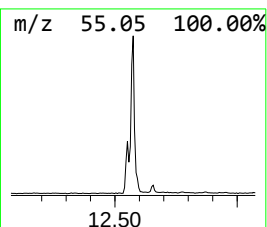
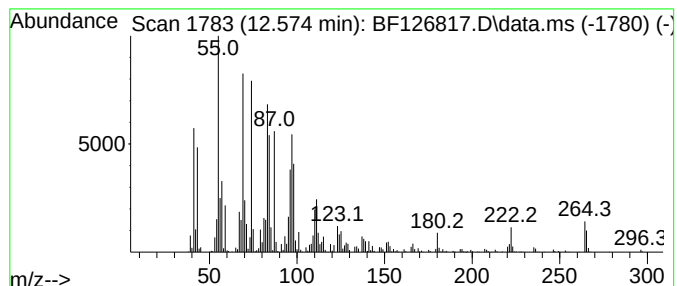
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 (Z)-15-Octadecenoic acid me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.574	57.21 ng	3850880	Phenanthrene-d10	11.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	93		
2	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	90		
3	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	86		
4	6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	70		
5	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	68		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020422\
Data File : BF126817.D
Acq On : 04 Feb 2022 18:05
Operator : CG/JU
Sample : N1381-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DB-09(25-30)-02-02-22

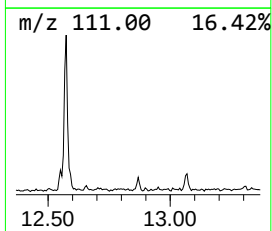
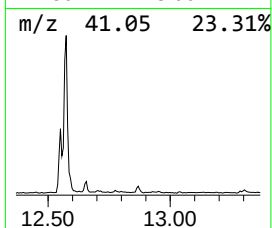
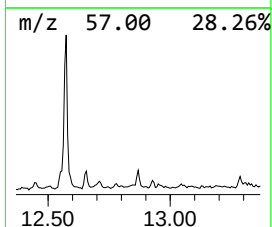
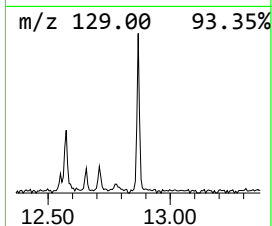
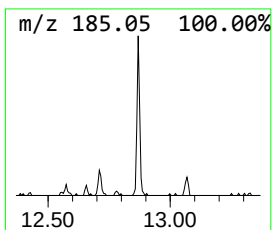
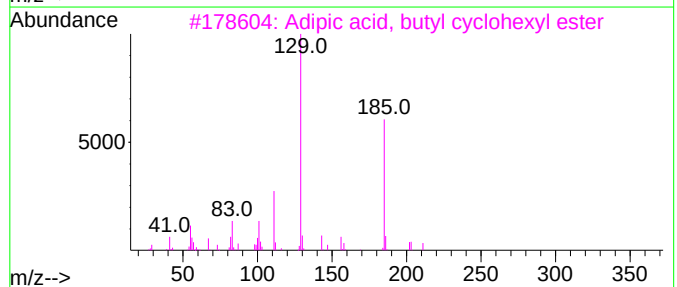
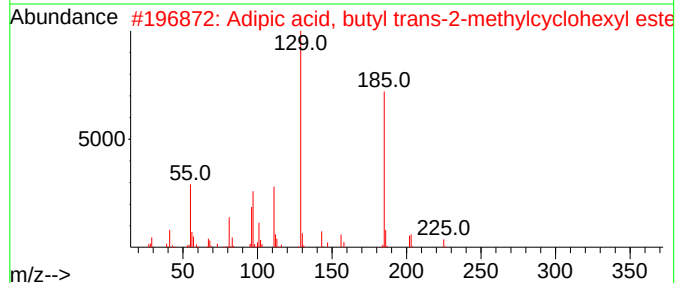
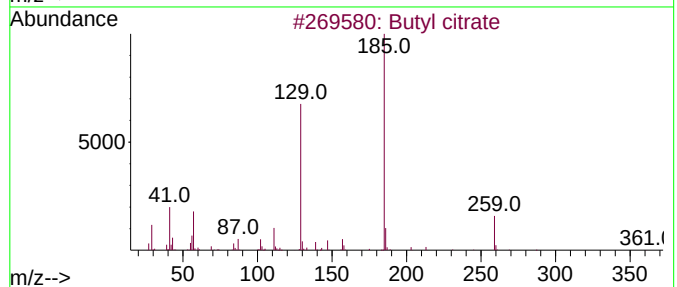
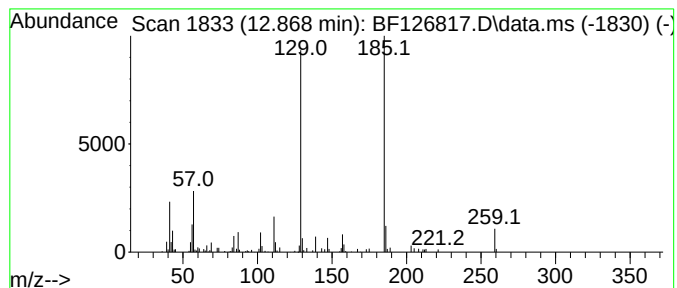
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Butyl citrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.868	2.57 ng	97235	Chrysene-d12	14.121

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl citrate	360	C18H32O7	000077-94-1	91
2			Adipic acid, butyl trans-2-methy...	298	C17H30O4	1000324-74-6	64
3			Adipic acid, butyl cyclohexyl ester	284	C16H28O4	1000324-25-9	64
4			Adipic acid, butyl 3-heptyl ester	300	C17H32O4	1010353-64-9	64
5			Adipic acid, butyl 3-hexyl ester	286	C16H30O4	1000353-62-3	56



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020422\
Data File : BF126817.D
Acq On : 04 Feb 2022 18:05
Operator : CG/JU
Sample : N1381-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DB-09(25-30)-02-02-22

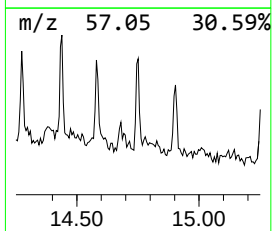
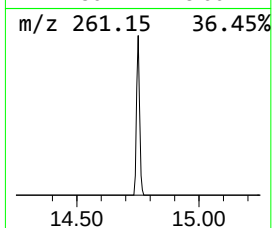
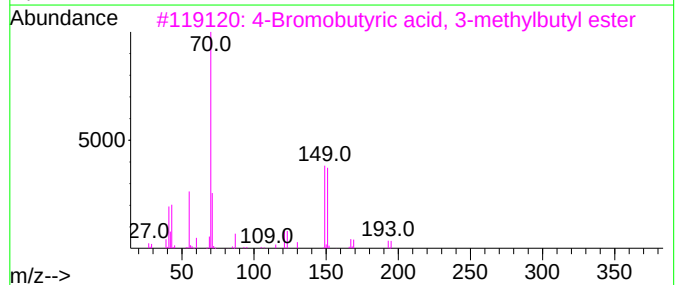
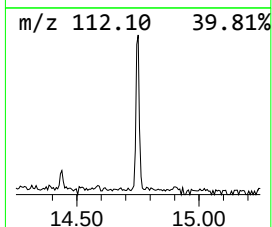
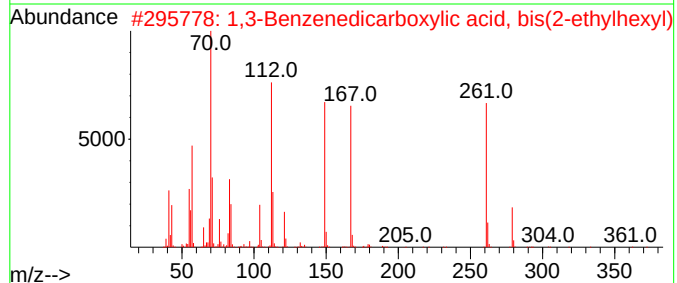
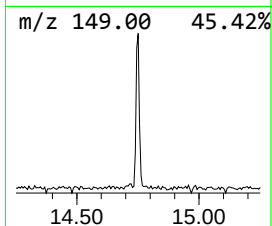
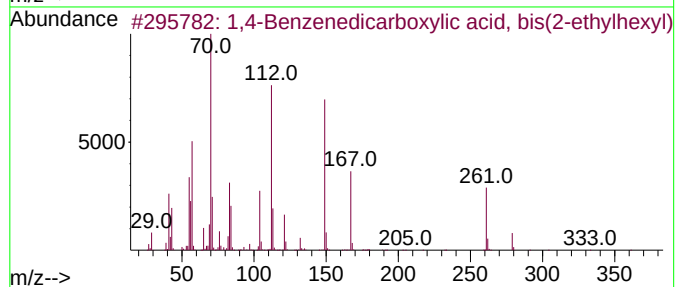
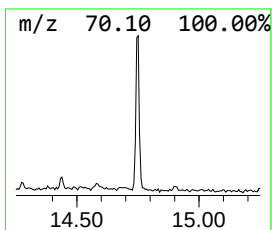
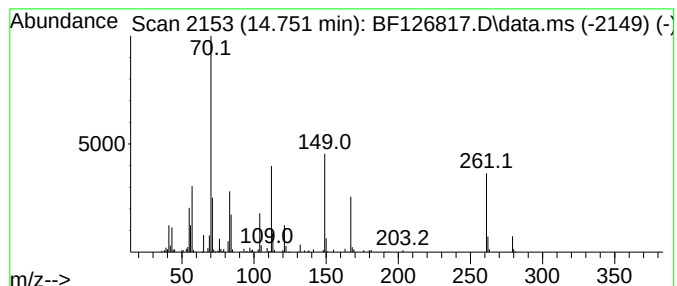
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1,4-Benzenedicarboxylic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.751	5.03 ng	190012	Chrysene-d12	14.121

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	62
2			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	52
3			4-Bromobutyric acid, 3-methylbut...	236	C9H17BrO2	1000354-68-4	37
4			1-(2-Hydroxymethylpyrrolidin-1-y...	143	C7H13NO2	1000192-83-2	25
5			Dimethylmalonic acid, monochlori...	262	C13H23ClO3	1000361-64-8	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020422\
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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DB-09(25-30)-02-02-22

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.299	13.0	ng	592302	1	6.945	908888	20.0
2-Ethylhexyl me...	9.575	2.2	ng	145025	3	9.986	1342240	20.0
Pentadecanoic a...	11.863	8.2	ng	548744	4	11.480	1346180	20.0
9,12-Octadecadi...	12.551	20.6	ng	1384340	4	11.480	1346180	20.0
(Z)-15-Octadece...	12.574	57.2	ng	3850880	4	11.480	1346180	20.0
Butyl citrate	12.868	2.6	ng	97235	5	14.121	755540	20.0
1,4-Benzenedica...	14.751	5.0	ng	190012	5	14.121	755540	20.0